Lattice QCD with dynamical domain wall quarks

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We study lattice QCD with two flavors of dynamical domain wall quarks. With renormalization group motivated actions, we find chiral symmetry can be preserved to a high degree at lattice cut off of $a^{-1} \sim 2$ GeV even for fifth dimension size as small as $L_s = 12$. In addition two new steps are introduced to improve the performance of the hybrid Monte Carlo simulation.

1. Introduction

An obvious source of systematic error in numerical lattice QCD at present is the quenched approximation. Use of domain wall fermion (DWF) [1] dynamical quarks to lift this approximation is attractive because DWF preserve the flavor and chiral symmetries both on and off shell on the lattice before the continuum limit is taken. Evidently successful implementation would bring many advantages, such as detailed study of flavor-singlet meson spectrum and its relation to the $U(1)_A$ anomaly. However some recent exploratory calculations [2] on coarse lattices with cut off of $a^{-1} < 1$ GeV show the chiral symmetry is rather poorly realized: impractically large $L_s \sim 100$ are necessary to bring the residual symmetry violation under control. In contrast in this work we go to a higher cutoff of $a^{-1} \sim 2$ GeV with renormalization-group (RG) motivated gauge actions and find that the residual violation can be made sufficiently small even at $L_s = 12$.

To cope with considerably larger demand for computing resources brought by this new approach, we introduce two improvements in the hybrid Monte Carlo (HMC) algorithm which accelerate the simulation reported below on the QCDSP by about a factor of three.

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2. New algorithms

The lattice QCD partition function with two flavors (N_F =2) of DWF quarks is

$$Z = \int \mathcal{D}U \frac{\det(D^\dagger D)|_{m=m_f}}{\det(D^\dagger D)|_{m=1}} e^{-S_g}, \tag{1}$$

where D is the 5d Dirac operator with 4d bare fermion mass m and S_g the gauge action. The determinant in the denominator in Eq. 1 comes from the Bosonic Pauli-Villars regulators, ϕ_{PV}, whose mass is set to 1 to cancel the dominating contribution from the fermions on the bulk 5d lattice. This allows us to study 4d QCD with 2 flavors of light quarks localized at the boundary and coupled to the 4d gauge field. The original fermion action employed in [3,2] was

$$\begin{aligned} S_F = \sum_{x,s} \{ & -\phi_F^\dagger (D^\dagger D)|_{m=m_f}^{-1} \phi_F \\ & -\phi_{PV}^\dagger (D^\dagger D)|_{m=1} \phi_{PV} \}, \end{aligned} \tag{2}$$

where ϕ_F is the pseudo-fermion field. By integrating out ϕ_F and ϕ_{PV}, we obtain the partition function Eq. 1. We chose hybrid Monte Carlo phi algorithm (HMC-ϕ) [4] to generate the Markov chain of gauge configurations.

Noticing equivalence between $\frac{\det(A^\dagger A)}{\det(B^\dagger B)}$ and $\{\det[B(A^\dagger A)^{-1} B^\dagger]\}^{-1}$, we could also obtain the partition function Eq. 1 from a new action [4]

$$S' = -\phi_F^\dagger [D|_{m=1} (D^\dagger D)|_{m=m_f}^{-1} D|_{m=1}^\dagger] \phi_F \tag{3}$$

[4]This part of the work is done mainly by C. Dawson.

where we need only one bosonic field ϕ_F. Even/odd preconditioning is implemented in either case.

The benefits of the new action and the associated force term are first the unwanted contribution from 5d bulk fermion is now canceled explicitly while it was canceled only stochastically in the original force term. This leads to better acceptance in the Metropolis accept/reject step, which increased by about 20% in a realistic simulation. Secondly, the source vector, ϕ_F, of the Dirac equation solved in the force term calculation is modified to $D^\dagger|_{m=1}\phi_F$ as seen in Eq. 3, and it turns out that the number of conjugate gradient(CG) iterations is 20 - 30 % smaller than that of the original action.

The second improvement [5] is to forecast the solution of the CG at each step of a HMD trajectory from the solutions of previous steps. In each of trajectories, the system obeys the smooth classical molecular dynamics (MD), so future solutions can be estimated from past ones. We choose the Minimal Residual Extrapolation method of [5] with a repeated Gram-Schmidt orthogonalization to ensure orthogonality. The solution is forecasted by minimizing the norm of the residual vector within the subspace spanned by previous solutions. Then the forecasted solution is passed into the ordinary CG as an initial input vector.

The manner of convergence of the CG based on different numbers of previous solutions in the forecasting is shown in Fig. 1. The squared norm of the residual vector of a solution (vertical axis) is already small, $\mathcal{O}(1)$, at zero CG count (horizontal axis) when the number of previous solution used in the forecast (N_p) is larger than one. The CG iterations required for convergence decreases monotonically with increasing N_p, up to 7.

The reversibility required to prove the detailed balance in the Markov chain is checked by flipping the sign of the conjugate momentum field at the end of a trajectory and evolving the configuration backward by the same number of MD steps. The resulting configuration obtained at the end of the reversed process differs from the initial configuration by less than 2×10^{-5} in elements of SU(3) link variables for a CG convergence criteria, $|res|/|src| < 10^{-8}$. By this trick with $N_p = 7$

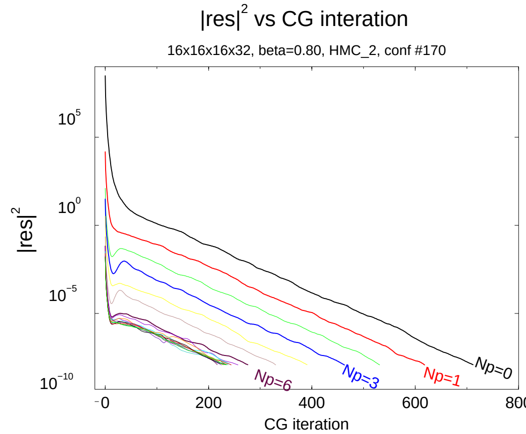

Figure 1. The squared norm of the residual vector as a function of CG steps. The initial solution vector is precognized based on previous N_p solutions.

the number of total CG count is 55 % of the original code (using $N_p = 1$) and about 35 % of a simulation without the forecasting.

3. Physical scale of the dynamical lattice

Observing the large chiral symmetry violation for coarser lattice spacing, $a^{-1} < 1$ GeV [2], we decided to perform a large scale simulation with target $a^{-1} \sim 2$ GeV. To quickly determine parameters for this target lattice spacing, we examined the parameter space on an $8^3 \times 4$ lattice and compared the meson spectrum to that obtained with the dynamical staggered fermions on the same lattice size assuming that scaling violations from the two fermion actions are mild. We also explored the dependence of the residual chiral symmetry breaking with various RG improved gauge actions. We found at fixed $a^{-1} \sim 2$ GeV that chiral symmetry was better realized for larger negative values of the coefficient of the (1×2) rectangular plaquette although the dependence of the residual mass, m_{res}, was much more mild than for quenched simulations [6].

For our most intensive simulation, we chose DBW2 gauge action at $\beta = 0.80$ with $N_F = 2$ on a $16^3 \times 32$ lattice. The sea quarks have mass $am_f^{(dyn)} = 0.02$, domain wall height $M_5 = 1.80$, and $L_s = 12$. An trajectory consists of 50 leapfrog steps and advances the MD time, τ, by 0.5.

The average number of CG iterations to fulfill the convergence criteria of $|res|/|src| < 10^{-8}$ is 550 for $N_p = 1$ and 314 for $N_p = 7$. The acceptance ratio of the accept/reject step is about 77(3) %. On a 4096 node partition ($\sim$ 205 GFLOPS peak) of the QCDSP, it takes about 1 hour per trajectory.

To estimate the lattice spacing within the statistics accumulated so far, we measure the heavy quark potential and the meson spectrum from the last 50 lattices which are separated by five trajectories after dropping the first 500 trajectories. We monitor the chiral condensate $\langle \bar{q}q \rangle$ as a function of the trajectory number and pick lattices for measurement after $\langle \bar{q}q \rangle$ is considered to have reached its thermalized value. However, we note that it is not clear whether the evolution is thermalized at this point.

Measuring the correlation between path ordered products of gauge-fixed links in the time direction of length T at a space point x, $L_T(x)$, we obtain the heavy quark potential $e^{-V(r)T} = \langle L_T^\dagger(x) L_T(x+r) \rangle$ [5]. As shown in Fig. 2, the fit to the data for $4 \le T \le 6$ and $\sqrt{2} \le r \le 7$ to the function $V(r) = C - \alpha/r + \sigma r$ gives $a\sqrt{\sigma} = 0.28(2)$, or $a^{-1} \approx 1.7(2)$ GeV, and the Sommer scale, $r_0/a = 4.1(3)$.

Meson propagators are calculated using valence quarks with $L_s = 12, M_5 = 1.8$ and $am_f^{(val)} = 0.015, 0.020, 0.025, 0.030$. Extrapolating the vector meson mass linearly, we find $aM_V(m_f^{(val)} \to 0)$ =0.34(9) which is consistent with the results of the heavy quark potential within (large) error. The squared mass of the pseudo-scalar meson is well fit to the PCAC relation. Taking the Kaon mass from experiment and the lattice spacing from the heavy quark potential yields a sea quark mass approximately half the strange quark mass.

Finally, the residual chiral symmetry breaking as determined from the pseudo-scalar mid-point correlator [7] turns out to be $am_{res}(m_f \to 0) = 1.47(7) \times 10^{-3}$, which corresponds to a few MeV.

[5]This calculation is done using the MILC code, version 6 for which we thank MILC collaboration.

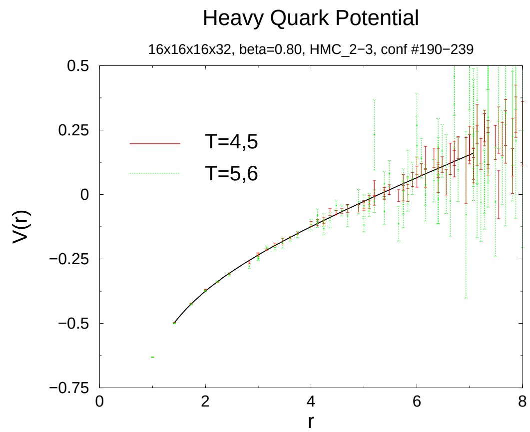

Figure 2. The heavy quark potential obtained from $T = 4 - 5$ (solid error bars) and $T = 5 - 6$ (dotted error bars) as a function of distance between quark and anti-quark with its fitted curve.

4. Conclusion and Discussion

In summary, we have begun investigating lattice QCD with two flavors of dynamical domain wall quarks. Assuming that the lattices have reached thermal equilibrium, we could interpret the configurations as QCD at roughly 0.1 fm lattice spacing, sea quarks with mass about $m_s/2$, and residual chiral symmetry breaking of only a few MeV. This level of symmetry breaking is now commensurate to that observed in quenched studies.

Two new algorithms were introduced to enhance the performance of the simulation. The speed up for the parameters discussed in this pilot study is about a factor of three. With this acceleration, further developments of theoretical and numerical techniques, and more computing horse power [8], we may reach our goal to study physics in the continuum limit of QCD.

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